Fumaric acid, pent-4-en-2-yl tridecyl ester

Inchi: InChI=1S/C22H38O4/c1-4-6-7-8-9-10-11-12-13-14-15-19-25-21(23)17-18-22(24)26-20(3
InchiKey: UBCSVUIMOSQVRF-ISLYRVAYSA-N
Formula: C22H38O4
SMILES: C=CCC(C)OC(=O)C=CC(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-167.86	kJ/mol	Joback Method
hf	-749.64	kJ/mol	Joback Method
hfus	53.71	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.905		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
tb	855.74	K	Joback Method
tc	1049.03	K	Joback Method
tf	460.18	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.32	J/mol×K	855.74	Joback Method
cpg	1056.35	J/mol×K	887.96	Joback Method
cpg	1073.29	J/mol×K	920.17	Joback Method
cpg	1089.18	J/mol×K	952.39	Joback Method
cpg	1104.05	J/mol×K	984.60	Joback Method
cpg	1117.95	J/mol×K	1016.82	Joback Method
cpg	1130.91	J/mol×K	1049.03	Joback Method
dvisc	0.0007412	Pa×s	460.18	Joback Method

dvisc	0.0003215	Pa×s	526.11	Joback Method
dvisc	0.0001680	Pa×s	592.03	Joback Method
dvisc	0.0000999	Pa×s	657.96	Joback Method
dvisc	0.0000654	Pa×s	723.89	Joback Method
dvisc	0.0000459	Pa×s	789.81	Joback Method
dvisc	0.0000340	Pa×s	855.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348932&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume